3,5-Dimethyl-3-heptanol

Inchi: InChI=1S/C9H20O/c1-5-8(3)7-9(4,10)6-2/h8,10H,5-7H2,1-4H3
InchiKey: NOSOEGQGQOMHBF-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCC(C)CC(C)(O)CC
Mol. weight [g/mol]: 144.26
CAS: 19549-74-7

Physical Properties

Property code	Value	Unit	Source
af	0.6066		Cheméo Relay (1.0)
gf	-111.52	kJ/mol	Joback Method
hf	-437.54	kJ/mol	Cheméo Relay (1.0)
hfus	12.22	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-2.14		Cheméo Relay (1.0)
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	445.52	K	Cheméo Relay (1.0)
tc	631.49	K	Cheméo Relay (1.0)
tf	241.72	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.46	J/mol×K	493.83	Joback Method
cpg	351.13	J/mol×K	522.34	Joback Method
cpg	364.17	J/mol×K	550.85	Joback Method
cpg	376.59	J/mol×K	579.36	Joback Method
cpg	388.42	J/mol×K	607.88	Joback Method
cpg	399.69	J/mol×K	636.39	Joback Method
cpg	410.41	J/mol×K	664.90	Joback Method

dvisc	0.1242076	Pa×s	239.43	Joback Method
dvisc	0.0170986	Pa×s	281.83	Joback Method
dvisc	0.0039538	Pa×s	324.23	Joback Method
dvisc	0.0012828	Pa×s	366.63	Joback Method
dvisc	0.0005256	Pa×s	409.03	Joback Method
dvisc	0.0002546	Pa×s	451.43	Joback Method
dvisc	0.0001397	Pa×s	493.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48309e+01
Coeff. B	-4.08303e+03
Coeff. C	-6.62500e+01
Temperature range (K), min.	347.00
Temperature range (K), max.	495.17

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549747&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume